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**EXAFS of the Low Spin Ferric Center of Nitrile Hydratase and Model Complexes**

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**ABSTRACT:** We have used X-ray spectroscopy to find structural evidence of ligand binding to the metal-centers of several  $\text{Fe}^{3+}$  and  $\text{Co}^{3+}$  coordination complexes that were designed to mimic the metalloenzyme Nitrile Hydratase (NHase). The ligands in these complexes (for example, 2,3,13,14-tetramethyl-4,8,12-triazapentadeca-3,12-diene-2,14-dithiol) coordinate through three nitrogen atoms and two thiolate sulfur atoms. Spectroscopic evidence existed supporting the binding of ligands such as acetonitrile and alcohols to the metal-centers of these compounds, however structural characterization proved to be impossible through methods other than XAS. The results obtained showed clear evidence for the binding of acetonitrile (NHase substrate) and methanol (model for the active-form of NHase) to three compounds of the ligand that spectroscopically mimicked the enzyme the best. Iron(III) complexes of a ligand that favors square pyramidal complexes (2,3,6,9,10-tetramethyl-6-nitrilomethyl-4,8-diazaundeca-3,8-diene-2,10-dithiol) were less reactive, adding a sixth ligand in acetonitrile but not in methanol.